Supporting Information

Regioselective, Transition Metal-Free C–O Coupling Reactions Involving Aryne Intermediates

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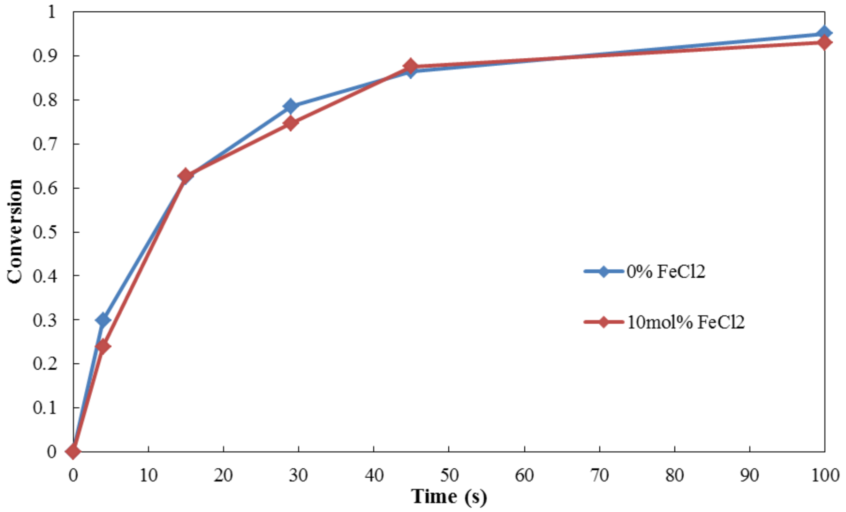
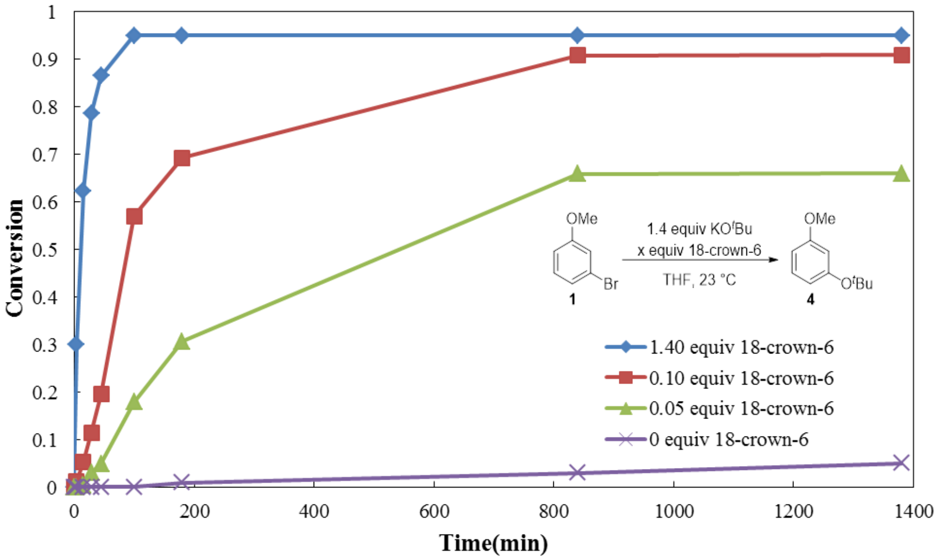
CONTENTS

1. **General Considerations:** Unless otherwise stated, all reactions and manipulations were carried out in a MBraun Labmaster glovebox or using standard Schlenk techniques under a nitrogen atmosphere. Hexanes, toluene, diethyl ether and ethyl acetate were purchased from Sigma Aldrich. Tetrahydrofuran was purchased from Macron Chemicals and dried using a JC Meyers Phoenix SDS solvent purification system. Potassium *tert*-butoxide was purchased from Sigma Aldrich (reagent grade and sublimed grade) and Strem and used both as received and sublimed. Sodium *tert*-butoxide was purchased from Sigma Aldrich and used as received. 3-Bromoanisole, 3-iodoanisole, 1-bromo-3-florobenzene, 1-iodo-3-florobenzene, 1-bromo-3-chlorobenzene, 1-bromo-2,5-dimethoxybenzene, 1-bromo-3,5-dimethoxybenzene, 1-chloro-3,5-dimethoxybenzene, 1-bromo-4,5-dimethoxybenzene, 2-bromo-4-fluoroanisole, 3-bromo-N,N-dimethylaniline and 1,4-dibromo-2-fluorobenzene were purchased from Sigma-Aldrich and used after passing through activated alumina and stored over activated molecular sieves overnight. Solid reagents were stored under high vacuum overnight prior to use. 18-Crown-6 was purchased from TCI and distilled before usage. 2-Bromo-1-fluoro-4-methoxybenzene was purchased from Oakwood Chemicals and used after passing through activated alumina and stored over activated molecular sieves overnight. 1-Bromo-4-chloro-2-fluorobenzene was purchased from TCI Chemicals and used after passing through activated alumina and stored over activated molecular sieves overnight. All NMR spectra were collected at ambient temperature (ca. 23°C) on Bruker AVQ-400, AV-500 or AV-600 NMR spectrometers, each equipped with a 5 mm BB probe, and referenced to the residual (proteo) solvent signals. The progresses of the reactions were monitored by ^{1}H NMR spectroscopy and yields determined by separated products. Products were isolated according to procedures described below.

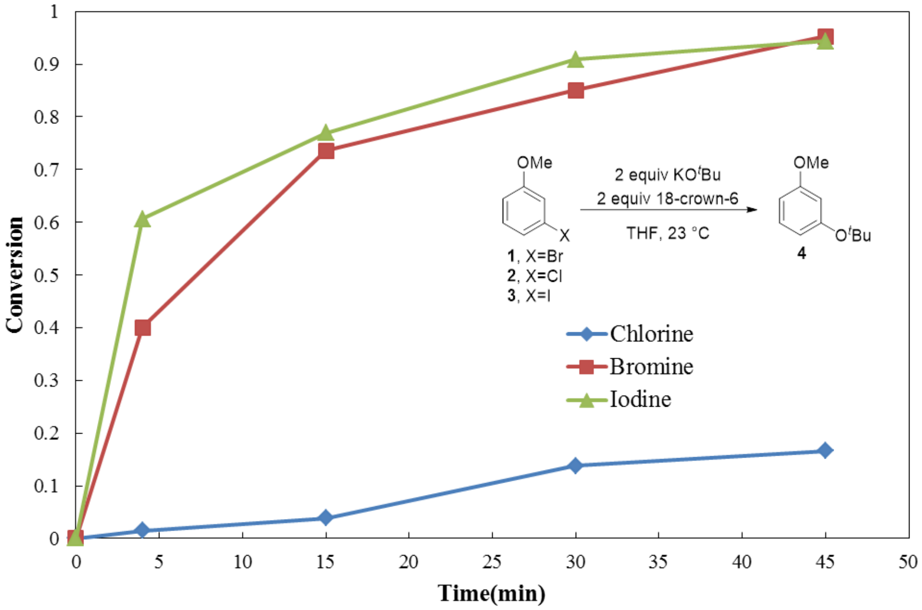
2. Supplementary Figures



Supplementary Figure 1. Conversion over time with or without extra $FeCl_2$ (conversion determined by ^{1}H NMR spectroscopy).

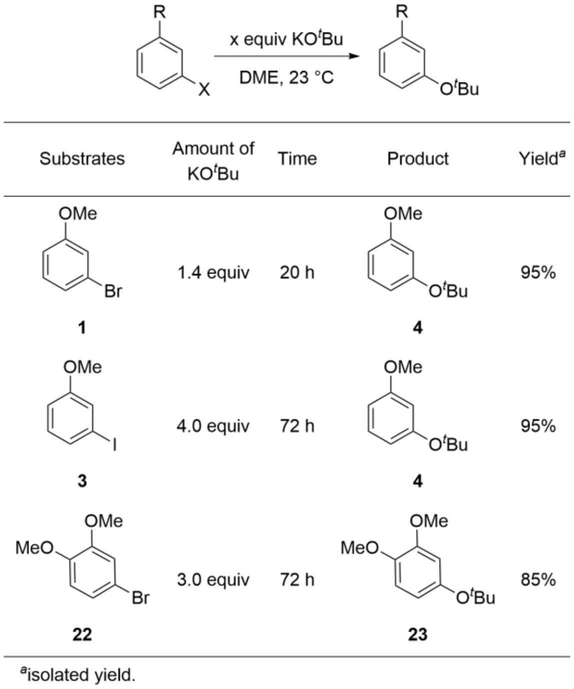


Supplementary Figure 2. Conversion over time with different amounts of 18-crown-6 (conversion determined by ^{1}H NMR spectroscopy).



Supplementary Figure 3. Conversion over time with different aryl halides (conversion determined by ^{1}H NMR spectroscopy).

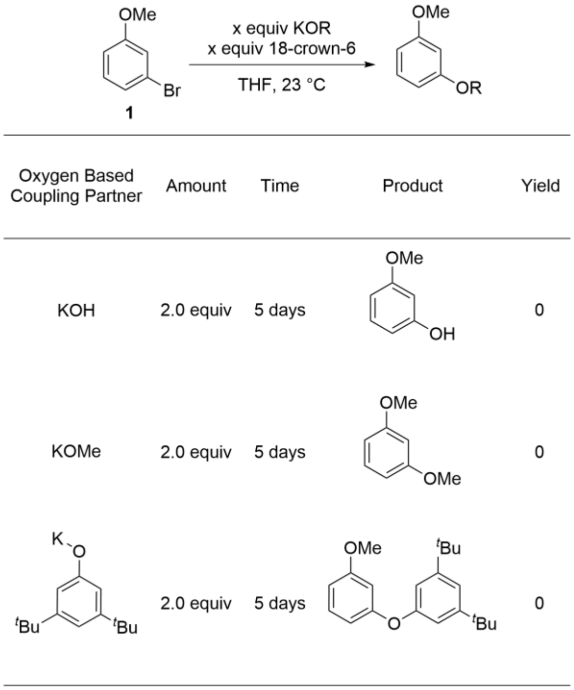
3. Supplementary Tables



Supplementary Table 1. Reactions Using DME as Solvent

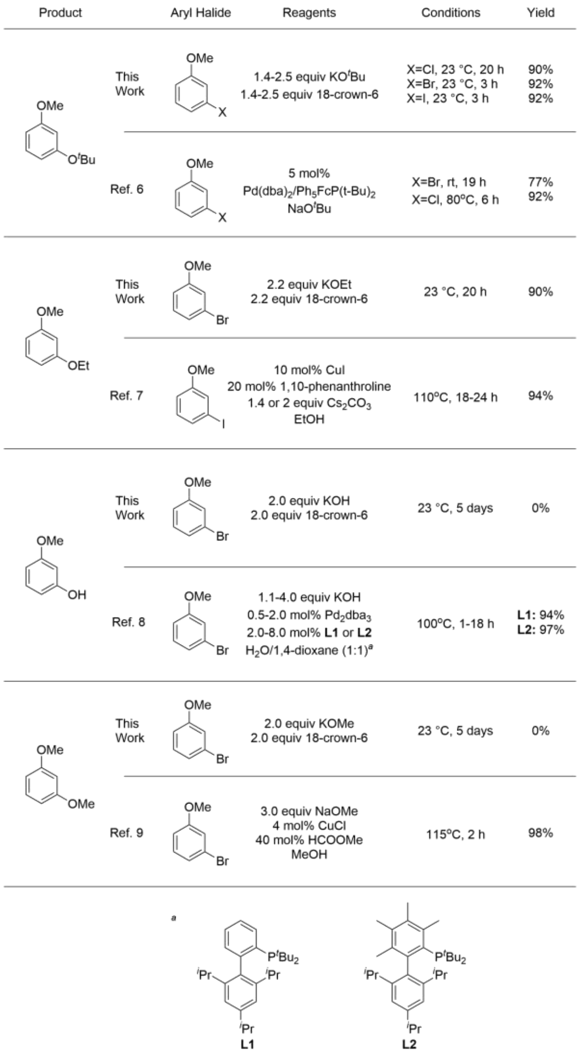
Substrates	Amount of KO^{t}Bu	Time	Product	Yield^a
1	1.4 equiv	20 h	4	95%
3	4.0 equiv	72 h	4	95%
22	3.0 equiv	72 h	23	85%

^{a}isolated yield.



Supplementary Table 2. Failed Oxygen-based Coupling Partners

Oxygen Based Coupling Partner	Amount	Time	Product	Yield
KOH	2.0 equiv	5 days		0
KOMe	2.0 equiv	5 days		0
	2.0 equiv	5 days		0



Product		Aryl Halide	Reagents	Conditions	Yield
OMe O^{t}Bu	This Work	OMe X	1.4-2.5 equiv KO^{t}Bu 1.4-2.5 equiv 18-crown-6	X=Cl, 23 °C, 20 h X=Br, 23 °C, 3 h X=I, 23 °C, 3 h	90% 92% 92%
	Ref. 6	OMe X	5 mol% Pd(dba)$_2$/Ph$_5$FcP(t-Bu)$_2$ NaO^{t}Bu	X=Br, rt, 19 h X=Cl, 80°C, 6 h	77% 92%
OMe OEt	This Work	OMe Br	2.2 equiv KOEt 2.2 equiv 18-crown-6	23 °C, 20 h	90%
	Ref. 7	OMe I	10 mol% CuI 20 mol% 1,10-phenanthroline 1.4 or 2 equiv Cs$_2$CO$_3$ EtOH	110°C, 18-24 h	94%
OMe OH	This Work	OMe Br	2.0 equiv KOH 2.0 equiv 18-crown-6	23 °C, 5 days	0%
	Ref. 8	OMe Br	1.1-4.0 equiv KOH 0.5-2.0 mol% Pd$_2$dba$_3$ 2.0-8.0 mol% **L1** or **L2** H$_2$O/1,4-dioxane (1:1)^a	100°C, 1-18 h	**L1:** 94% **L2:** 97%
OMe OMe	This Work	OMe Br	2.0 equiv KOMe 2.0 equiv 18-crown-6	23 °C, 5 days	0%
	Ref. 9	OMe Br	3.0 equiv NaOMe 4 mol% CuCl 40 mol% HCOOMe MeOH	115°C, 2 h	98%

Supplementary Table 3. Comparisons with Transition-metal Catalyzed C–O Couplings

4. **General C–O Coupling Procedure:** To a 20 mL scintillation vial was added aryl halide (Supplementary Table 4) and 5 mL of THF. To another 20 mL scintillation vial was added potassium *tert*-butoxide (amount specified in Table 1), 18-crown-6 (amount specified in Table 1), and 5 mL of THF. The solution from the first vial was then added to the second vial *via* pipette, with stirring. The reaction was stopped after a certain time period as listed in Tables 1 and 2, by quenching with wet diethyl ether. The product was separated using the procedures below. Yields were determined based on the mass of the purified product.

Supplementary Table 4. Amount of Starting Materials Used

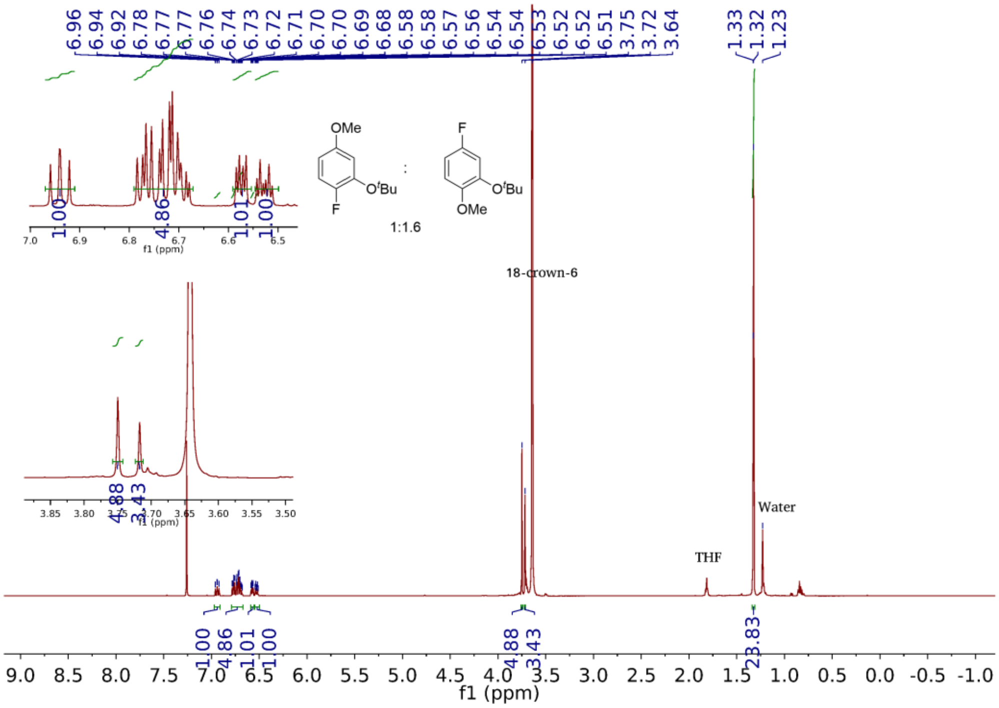
Compound	Mass(g)	Mol(mmol)		Compound	Mass(g)	Mol(mmol)
1	0.30	1.6		**19**	0.24	1.4
2	0.23	1.6		**20**	0.30	1.4
3	0.38	1.6		**22**	0.30	1.4
14	0.28	1.6		**24**	0.30	1.6
16	0.36	1.6		**26**	0.30	1.5
17	0.30	1.4				

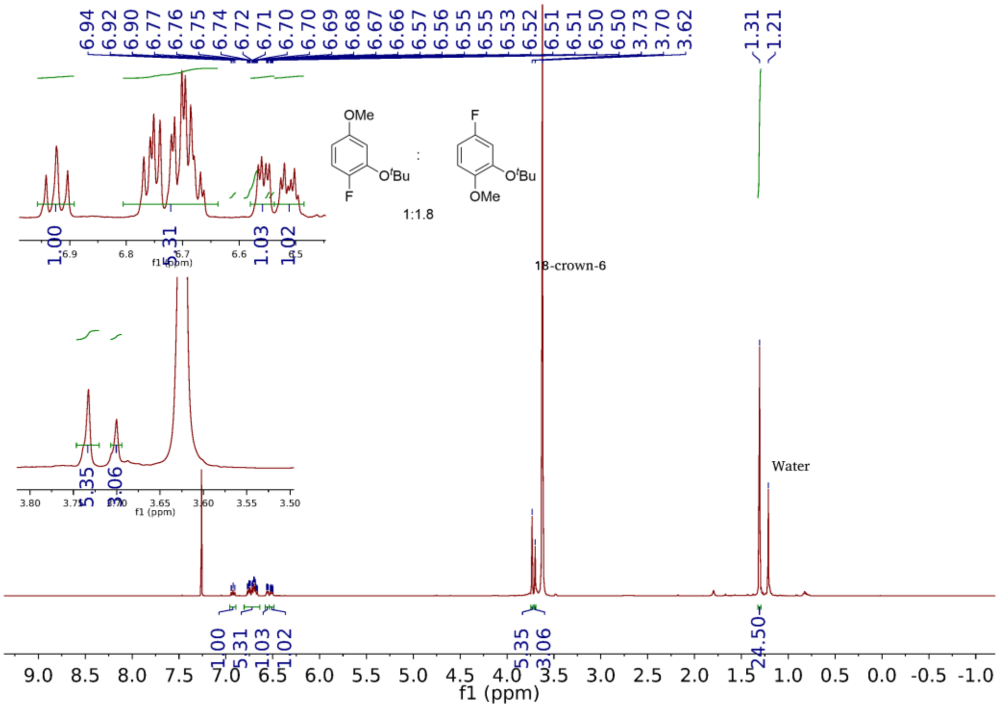
5. **Preparation procedure for 30:** To a 20 mL scintillation vial was added aryl halide (**28** or **29**, 0.10 g) and 9 mL of THF. To another 20 mL scintillation vial was added potassium *tert*-butoxide (amount specified in Table 1), 18-crown-6 (amount specified in Table 1), and 9 mL of THF. The solution from the first vial was then added to the second vial *via* pipette, with stirring. The reaction was stopped after a certain time period as listed in Tables 1, by quenching with wet diethyl ether. The product was separated using the procedures below. Yields were determined based on the mass of the purified product.

6. **Preparation procedure for 41:** To a 20 mL scintillation vial was added potassium *tert*-butoxide (0.25 g, 2.2 mmol), 18-crown-6 (0.59 g, 2.2 mmol), and 5 mL of THF. A solution of N-methylaniline (0.24 g, 2.2 mmol) in 5 mL of THF was added to the vial with stirring. After 5 min, a solution of 3-bromoanisole (0.30 g, 1.6 mmol) in 5 mL of THF was slowly added to the vial. The reaction mixture was allowed to stir for 20 h, and was then quenched with wet diethyl ether. The product was purified using silica column chromatography (toluene:hexanes, 1:9) and isolated as a white solid (0.28 g, 82%).

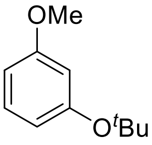
7. **Procedure for Constructing Supplementary Figures 2 and 3:** To a 20 mL scintillation vial was added aryl halide (30 mg), hexamethylbenzene (ca. 6 mg), and 3 mL of THF. To another 20 mL scintillation vial was added potassium *tert*-butoxide (amount specified in Supplementary Figures 2 and 3), 18-crown-6 (amount specified in Supplementary Figures 2 and 3), and 4 mL of THF. The solution from the first vial was then added to that of the second vial *via* pipette, with stirring. Conversions were determined by taking aliquots at 4, 15, 29, 100, 180, 840, and 1380 min, and quenching the aliquot with wet diethyl ether. The amount of product was determined using ^{1}H NMR spectroscopy to integrate the product signals against the hexamethylbenzene internal standard.

8. Evidence for Scheme 5

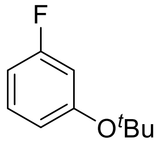




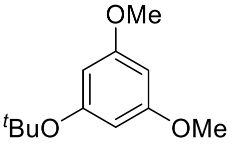
9. Characterization Data



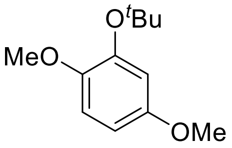
1-(tert-butoxy)-3-methoxybenzene (4). The product was purified using a 20 cm^3 silica plug washed with hexanes, and was isolated as a colorless oil (From **1**: 0.27 g, 92%; from **2**: 0.26 g, 90%; from **3**: 0.27 g, 92%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.16 (t, *J* = 8.2 Hz, 1H), 6.65-6.63 (m, 1H), 6.63-6.60 (m, 1H), 6.56 (t, *J* = 2.2 Hz 1H), 3.78 (s, 3H), 1.36 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.3, 156.8, 129.2, 116.5, 110.2, 108.9, 78.6, 55.3, 29.0.



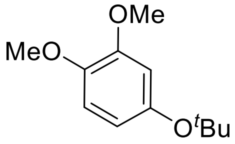
1-(tert-butoxy)-3-fluorobenzene (15). The product was purified using a 20 cm^3 silica plug washed with hexanes, and was isolated as a colorless oil (From **14**: 0.25 g, 92%; from **16**: 0.24 g, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (q, *J* = 8.0 Hz, 1H), 6.80-6.78 (m, 2H), 6.74-6.71 (m, 1H), 1.37 (s, 9H).; ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9 (d, *J* = 245.6 Hz), 156.9 (d, *J* = 10.5 Hz), 129.4 (d, *J* = 10.0 Hz), 119.5 (d, *J* = 3.0 Hz), 111.2 (d, *J* = 21.8 Hz), 110.0 (d, *J* = 21.1 Hz), 79.1, 28.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.7 (q, *J* = 8.6 Hz).



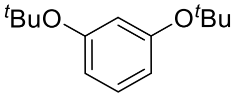
1-(tert-butoxy)-3,5-dimethoxybenzene (18). The product was purified using a 20 cm^3 silica plug washed with hexanes, and was isolated as a pale yellow oil (From **17**: 0.25 g, 86%; from **19**: 0.24 g, 83%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.21 (t, *J* = 2.1 Hz, 1H), 6.17 (d, *J* = 2.1 Hz, 2H), 3.76 (s, 6H), 1.37 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.9, 157.5, 102.5, 95.7, 78.9, 55.5, 29.1; HRMS (EI, m/z): Calcd for $C_{12}H_{18}O_3$ $[M\cdot]^+$ 210.1256, found 210.1259.



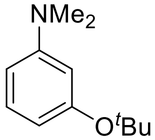
1-(tert-butoxy)-2,4-dimethoxybenzene (21). The product was purified using a 20 cm^3 silica plug washed with hexanes, and was isolated as a pale yellow oil (0.25 g, 86%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.81 (d, *J* = 8.8 Hz, 1H), 6.63 (d, *J* = 3.0 Hz, 1H), 6.58 (dd, *J* = 8.8, 3.0 Hz, 1H), 3.77 (s, 3H), 3.75 (s, 3H), 1.36 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.7, 148.7, 145.7, 113.4, 112.7, 108.2, 80.2, 56.6, 55.8, 28.8; HRMS (EI, m/z): Calcd for $C_{12}H_{18}O_3$ $[M\cdot]^+$ 210.1256, found 210.1260.



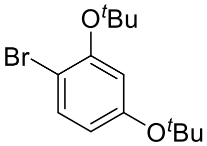
4-(tert-butoxy)-1,2-dimethoxybenzene (23). The product was purified using a 20 cm^3 silica plug washed with hexanes, and was isolated as a pale yellow oil (0.23 g, 79%). ^{1}H NMR (600 MHz, CDCl$_3$) δ 6.74 (d, *J* = 8.2 Hz, 1H), 6.55 (s, 1H), 6.53 (dd, *J* = 8.2, 2.6 Hz, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 1.32 (s, 9H); ^{13}C NMR (150 MHz, CDCl$_3$) δ 149.1, 148.9, 145.5, 115.7, 110.9, 109.0, 78.4, 56.2, 56.0, 28.9; HRMS (EI, m/z): Calcd for $C_{12}H_{18}O_3$ [M·]$^+$ 210.1256, found 210.1259.



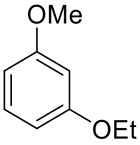
1,3-di-tert-butoxybenzene (25). The product was purified using a 20 cm^3 silica plug washed with hexanes, and was isolated as a colorless oil (0.25 g, 73%). ^{1}H NMR (600 MHz, CDCl$_3$) δ 7.12 (t, *J* = 8.1 Hz, 1H), 6.73 (dd, *J* = 8.1, 2.3 Hz, 2H), 6.65 (t, *J* = 2.3 Hz, 1H), 1.33 (s, 18H); ^{13}C NMR (150 MHz, CDCl$_3$) δ 155.8, 128.3, 120.3, 119.3, 78.5, 28.9; HRMS (EI, m/z): Calcd for $C_{14}H_{22}O_2$ [M·]$^+$ 222.1620, found 222.1617.



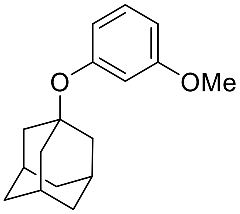
3-(tert-butoxy)-N,N-dimethylaniline (27). The product was purified using preparation TLC plate (toluene:hexanes 1:9), and was isolated as a colorless oil (0.16 g, 55%). ^{1}H NMR (500 MHz, CDCl$_3$) δ 7.11 (t, *J* = 8.1 Hz, 1H), 6.48 (dd, *J* = 8.3, 2.5 Hz, 1H), 6.39 (dd, *J* = 8.0, 2.1 Hz, 1H), 6.37 (t, *J* = 2.3 Hz, 1H), 2.92 (s, 6H), 1.36 (s, 9H). ^{13}C NMR (150 MHz, CDCl$_3$) δ 156.5, 151.7, 129.0, 112.5, 109.1, 108.0, 78.2, 40.8, 29.2; HRMS (EI, m/z): Calcd for $C_{12}H_{19}NO$ [M·]$^+$ 193.1467, found 193.1467.



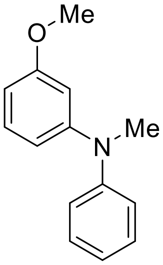
1-bromo-2,4-di-tert-butoxybenzene (30). The product was purified using preparation TLC plate (pre-neutralized using basic eluent; for **28**: toluene:hexanes:triethylamine 10:90:1; for **29**: toluene:hexanes:triethylamine 50:50:1), and was isolated as a colorless oil (from **28**: 0.04 g, 35%; from **29**: 0.03 g, 22%). ^{1}H NMR (500 MHz, CDCl$_3$) δ 7.40 (d, *J* = 8.7 Hz, 1H), 6.78 (d, *J* = 2.6 Hz, 1H), 6.61 (dd, *J* = 8.6, 2.6 Hz, 1H), 1.43 (s, 9H), 1.33 (s, 9H); ^{13}C NMR (150 MHz, CDCl$_3$) δ 155.2, 153.5, 132.6, 120.4, 120.2, 113.3, 81.6, 79.2, 29.2, 29.0; HRMS (EI, m/z): Calcd for $C_{14}H_{21}BrO_2$ [M·]$^+$ 300.0725, found 300.0727.



1-ethoxy-3-methoxybenzene (33). The product was purified using a 20 cm^3 silica plug washed with hexanes, and was isolated as a colorless oil (0.22 g, 90%). ^{1}H NMR (600 MHz, CDCl$_3$) δ 7.18 (t, *J* = 8.2 Hz, 1H), 6.51 (dd, *J* = 8.2, 2.4 Hz, 2H), 6.48 (t, *J* = 2.4 Hz, 1H), 4.03 (q, *J* = 7.0 Hz, 2H), 3.80 (s, 3H), 1.42 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (150 MHz, CDCl$_3$) δ 160.9, 160.3, 130.0, 106.8, 106.2, 101.0, 63.5, 55.4, 15.0.



3-(tert-butoxy)phenoxyadamantane (35). The product was purified using silica column chromatography (ethyl acetate:hexanes 1:9) and was isoalted as a colorless oil (0.35 g, 85%). ^{1}H NMR (600 MHz, CDCl$_3$) δ 7.15 (t, *J* = 8.1 Hz, 1H), 6.67-6.65 (m, 1H), 6.61-6.59 (m, 1H), 6.56 (t, *J* = 2.3 Hz, 1H), 3.78 (s, 3H), 2.17 (m, 3H), 1.88 (m, 6H), 1.64-1.58 (m, 6H); ^{13}C NMR (150 MHz, CDCl$_3$) δ 160.2, 155.5, 129.0, 117.5, 111.1, 109.3, 78.0, 55.4, 43.0, 36.3, 31.0; HRMS (EI, m/z): Calcd for $C_{17}H_{22}O_2$ [M·]$^+$ 258.1620, found 258.1623.

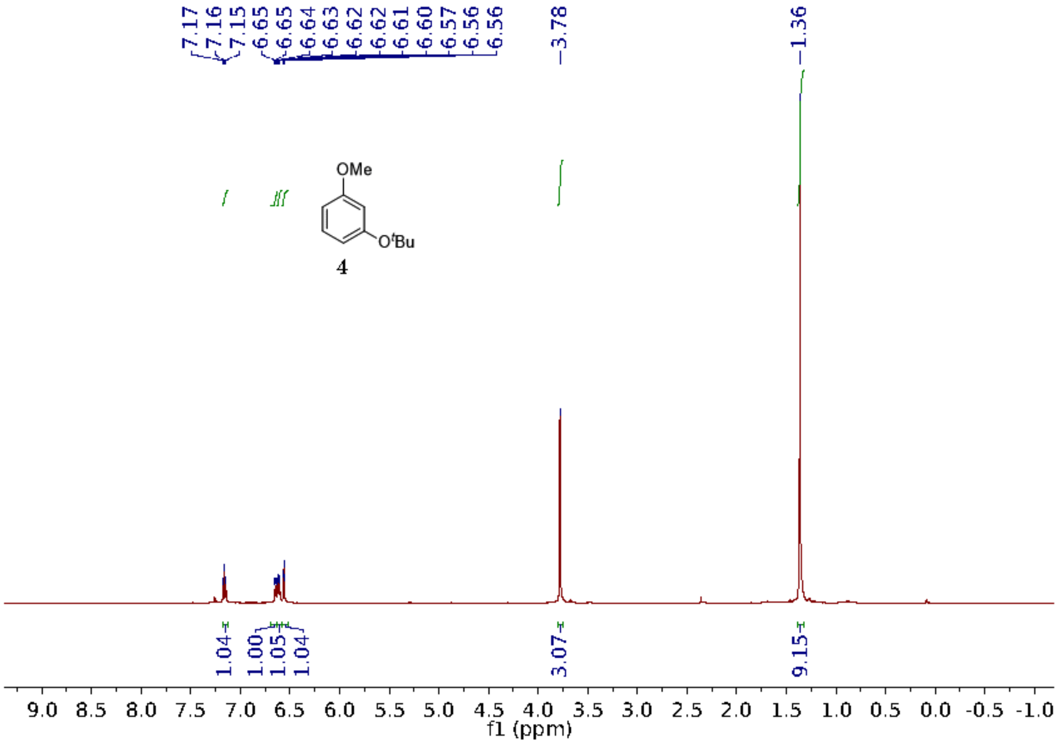


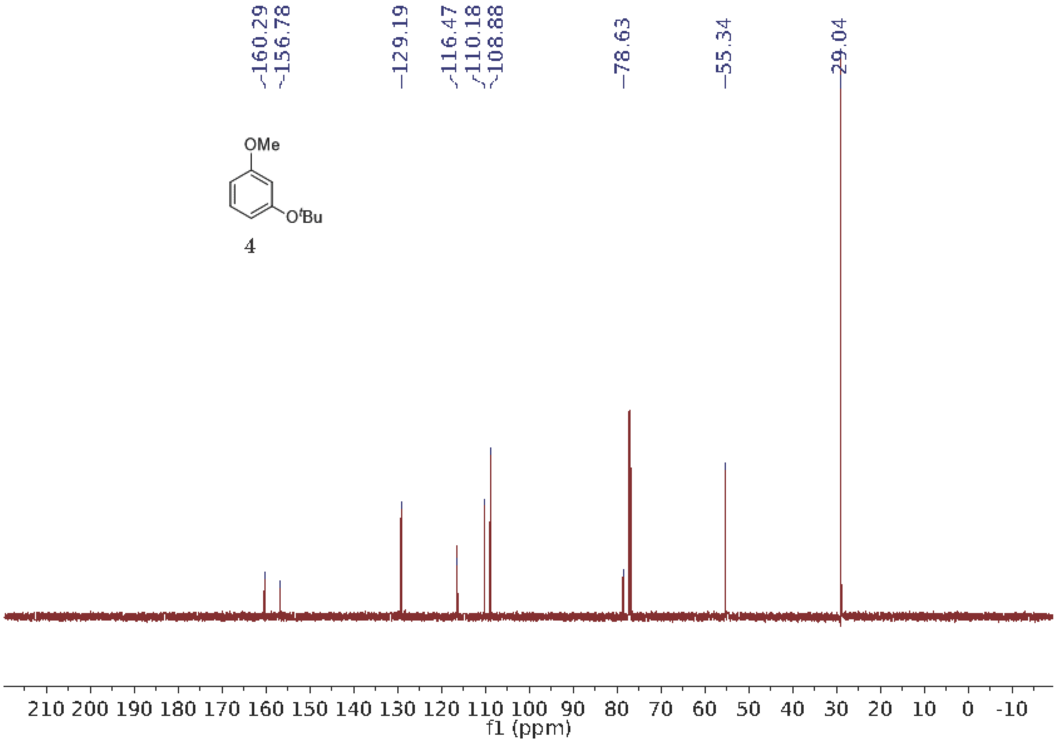
3-methoxy-N-methyl-N-phenylaniline (41). The product was purified using silica column chromatography (toluene:hexanes, 1:9) and isolated as a white solid (0.28 g, 82%). ^{1}H NMR (600 MHz, CDCl$_3$) δ 7.33-7.31 (m, 2H), 7.19 (t, *J* = 8.1 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 2H), 7.03 (t, *J* = 7.3 Hz, 1H), 6.62-6.61 (m, 1H), 6.58 (t, *J* = 2.2 Hz, 1H), 6.53-6.51 (m, 1H), 3.79 (s, 3H), 3.34 (s, 3H); ^{13}C NMR (150 MHz, CDCl$_3$) δ 160.5, 150.4, 148.8, 129.8, 129.2, 122.0, 121.6, 112.2, 105.9, 105.6, 55.2, 40.3.

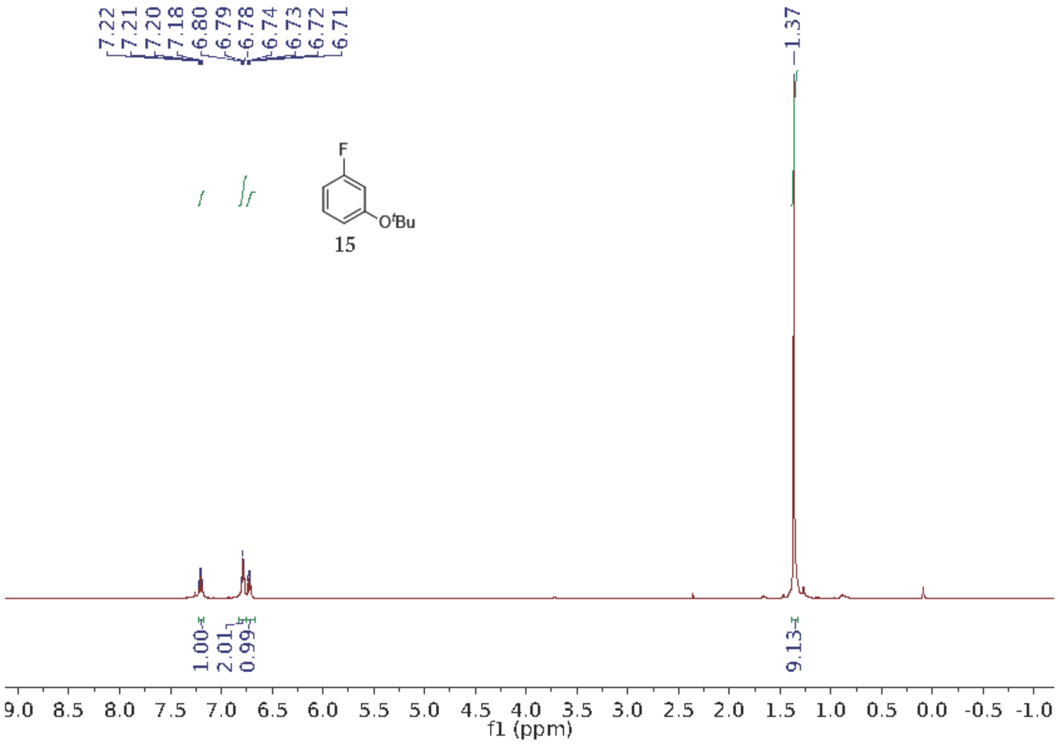
1-(tert-butoxy)-3-methoxybenzene (4), 1-(tert-butoxy)-3-fluorobenzene (15), 1-ethoxy-3-methoxybenzene (*33*), *3-(tert-butoxy)phenoxyadamantane (35)* and *3-methoxy-N-methyl-N-phenylaniline (41)* are known compounds.[1,2,3,4]

10. ^{1}H, ^{13}C and ^{19}F NMR Spectra of the Products

(All spectra were taken in $CDCl_3$.)



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7.21
7.20
7.18
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6.79
6.78
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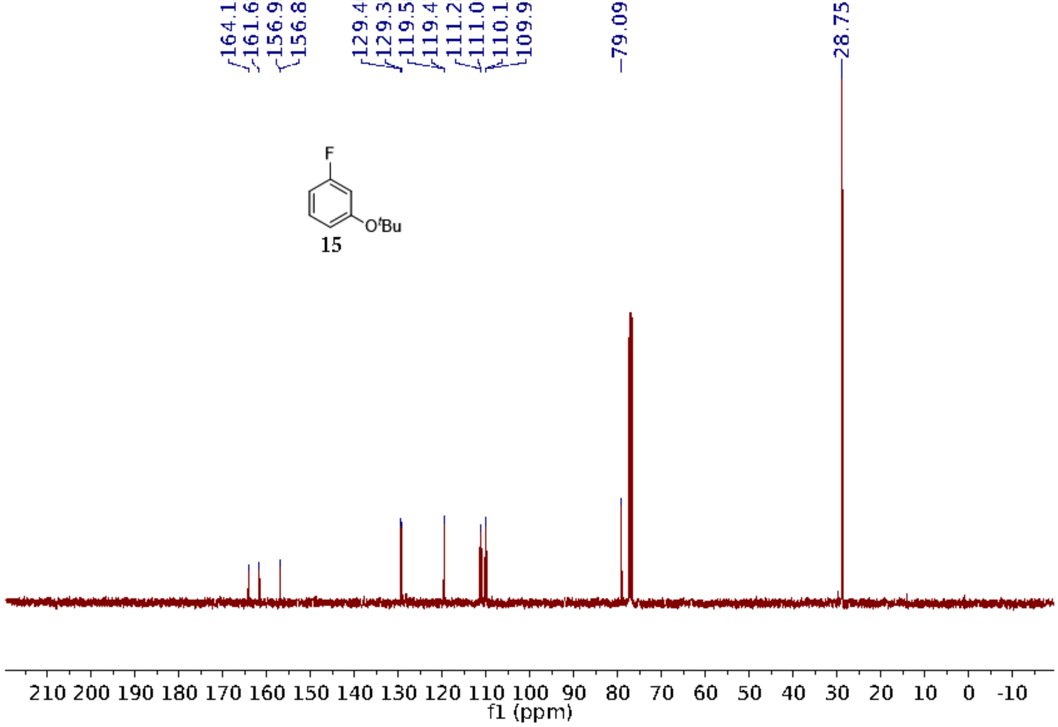
6.73
6.72
6.71
1.37
F
O^{t}Bu
15
1.00
2.01
0.99
9.13
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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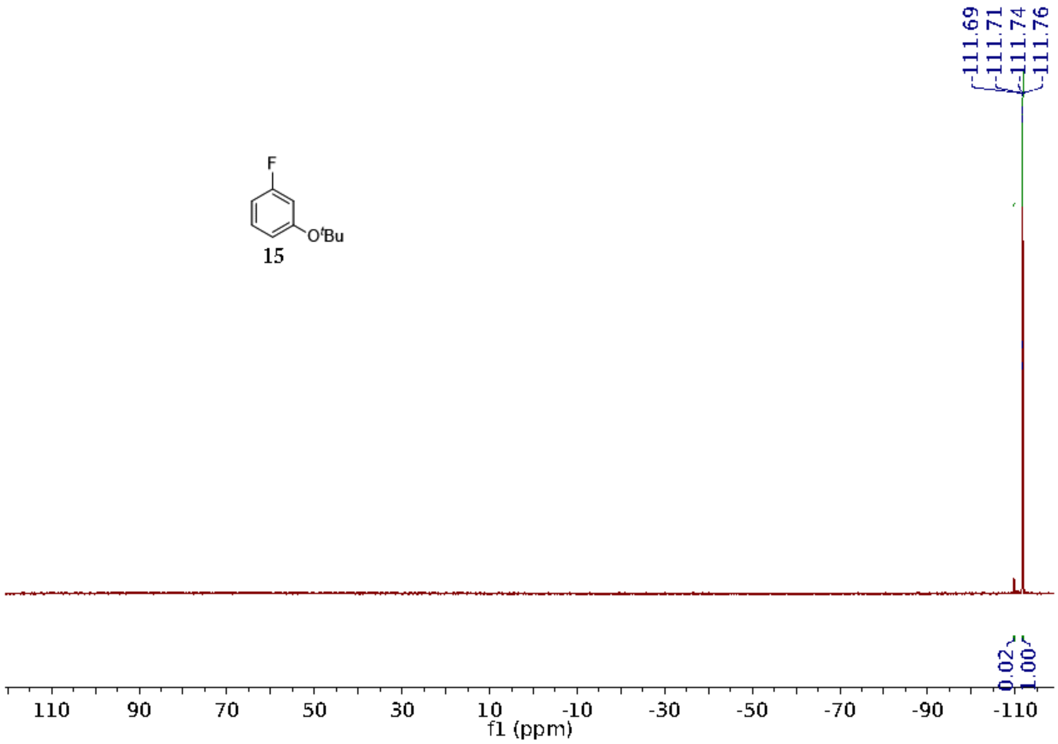
156.95
156.84
129.40
129.30
119.50
119.47
111.28
111.06
110.13
109.92
79.09
28.75
F
O^{t}Bu
15
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-111.69
-111.71
-111.74
-111.76
F
O^tBu
15
0.02
1.00
110
90
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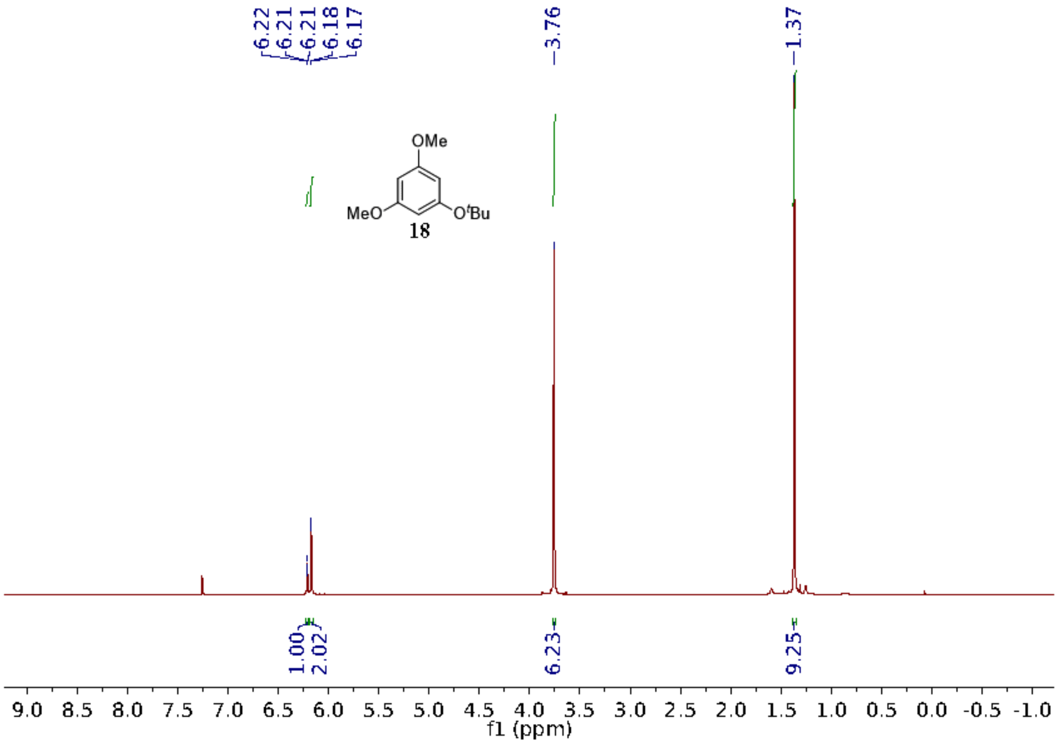
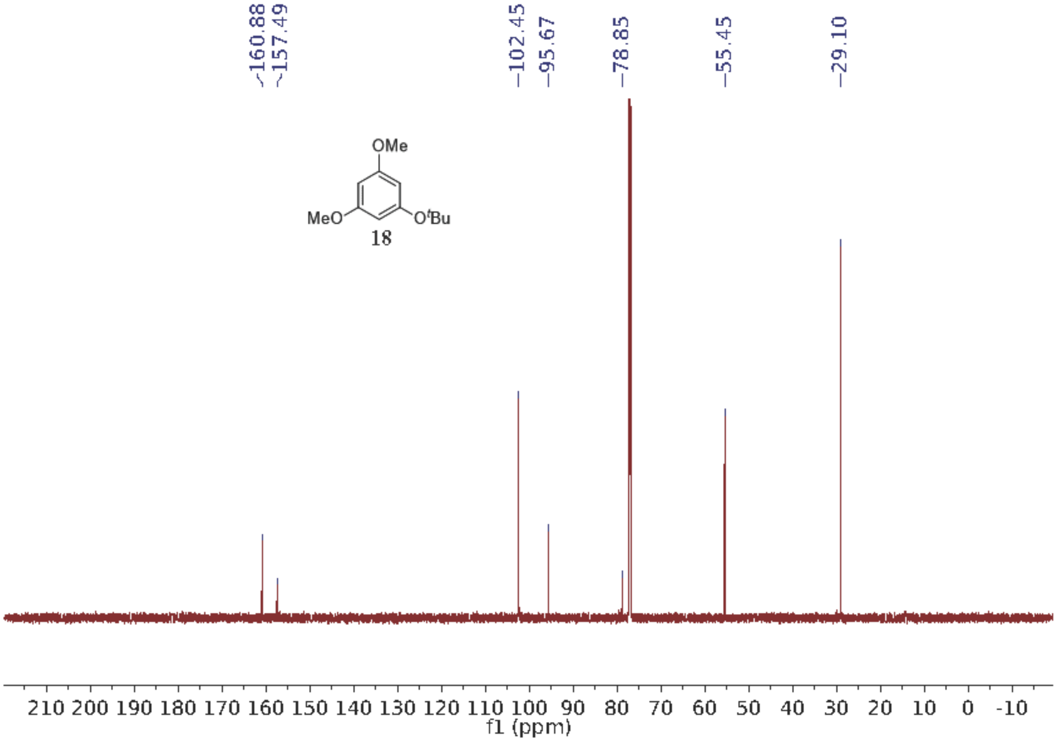
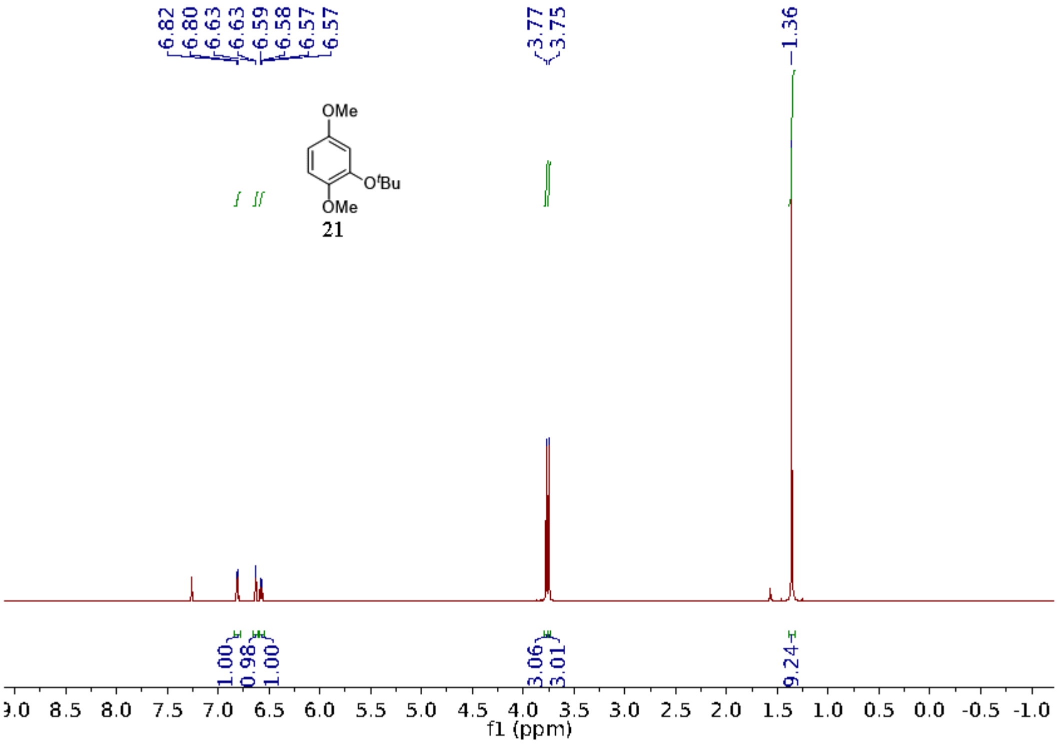
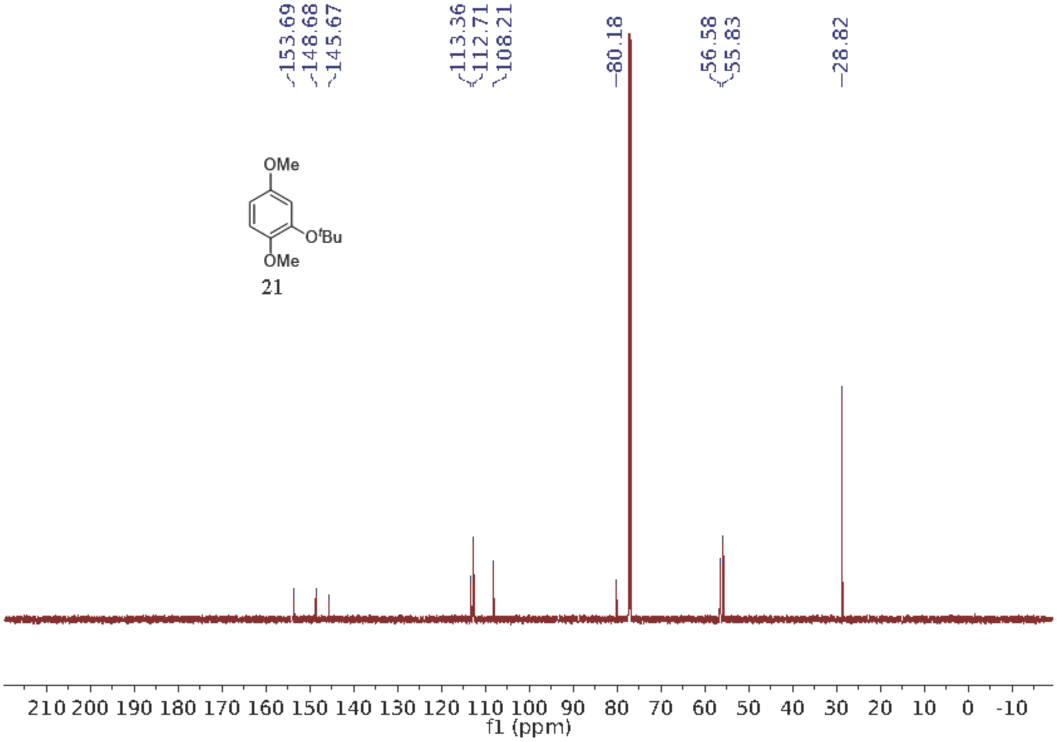
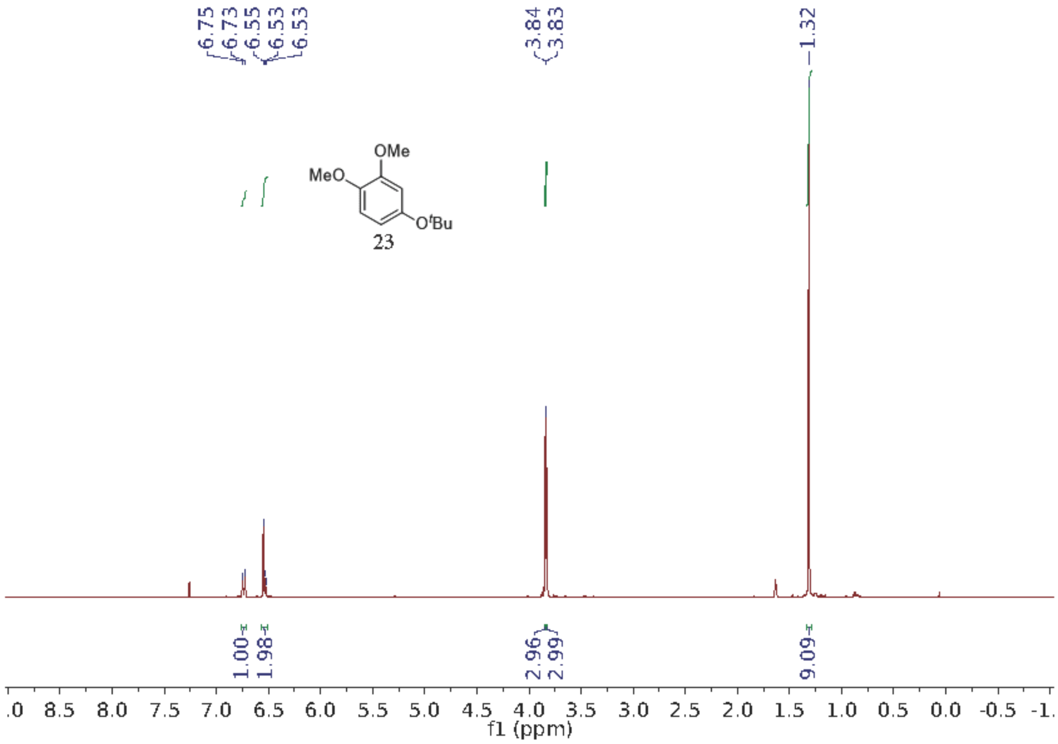
50
30
10
-10
-30
-50
-70
-90
-110
f1 (ppm)

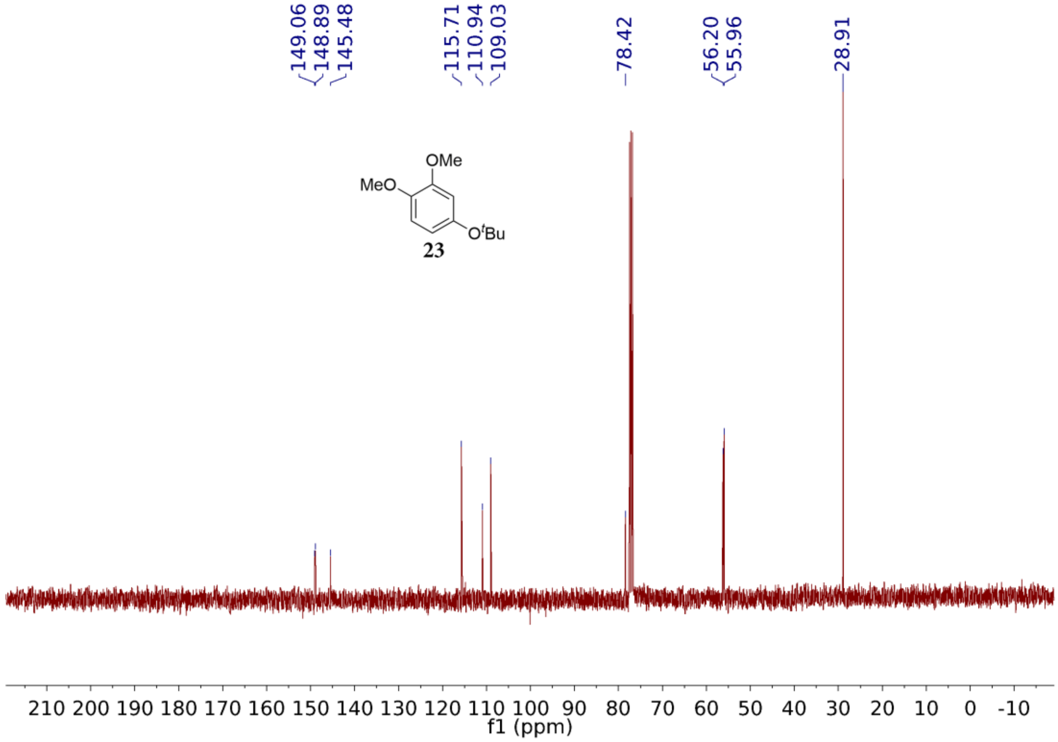

6.22
6.21
6.21
6.18
6.17
3.76
1.37
OMe
MeO
O^{t}Bu
18
1.00
2.02
6.23
9.25
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

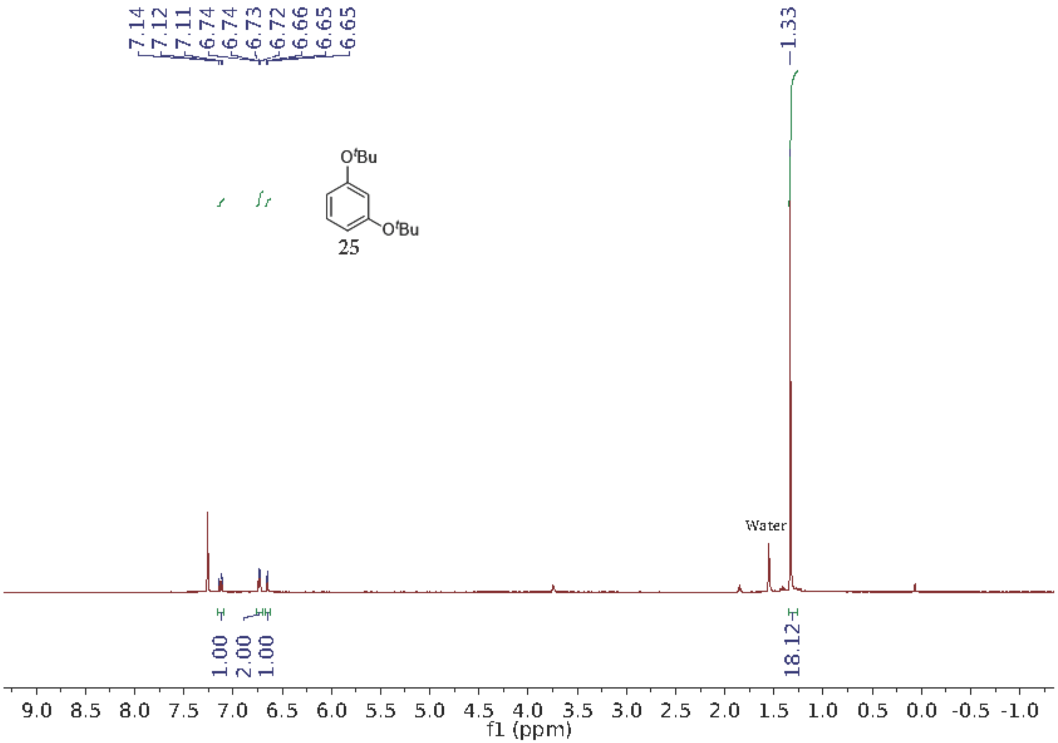

160.88
157.49
102.45
95.67
78.85
55.45
29.10
OMe
MeO
O^{t}Bu
18
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

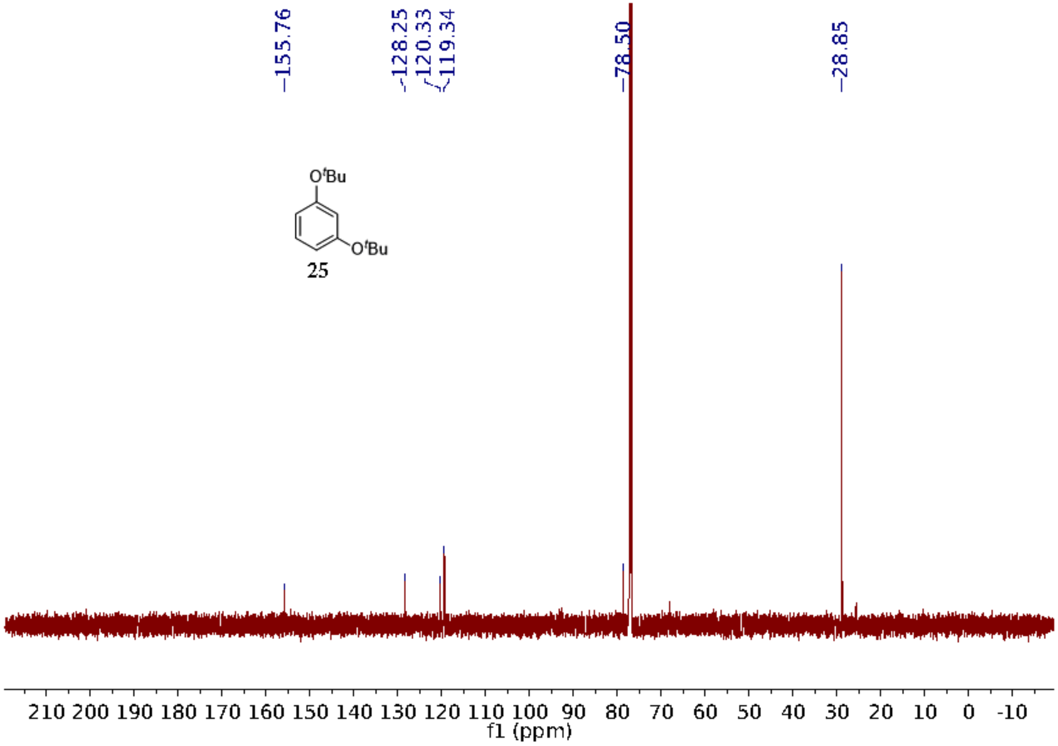

6.82
6.80
6.63
6.63
6.59
6.58
6.57
6.57
3.77
3.75
1.36
OMe
O^{t}Bu
OMe
21
1.00
0.98
1.00
3.06
3.01
9.24
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

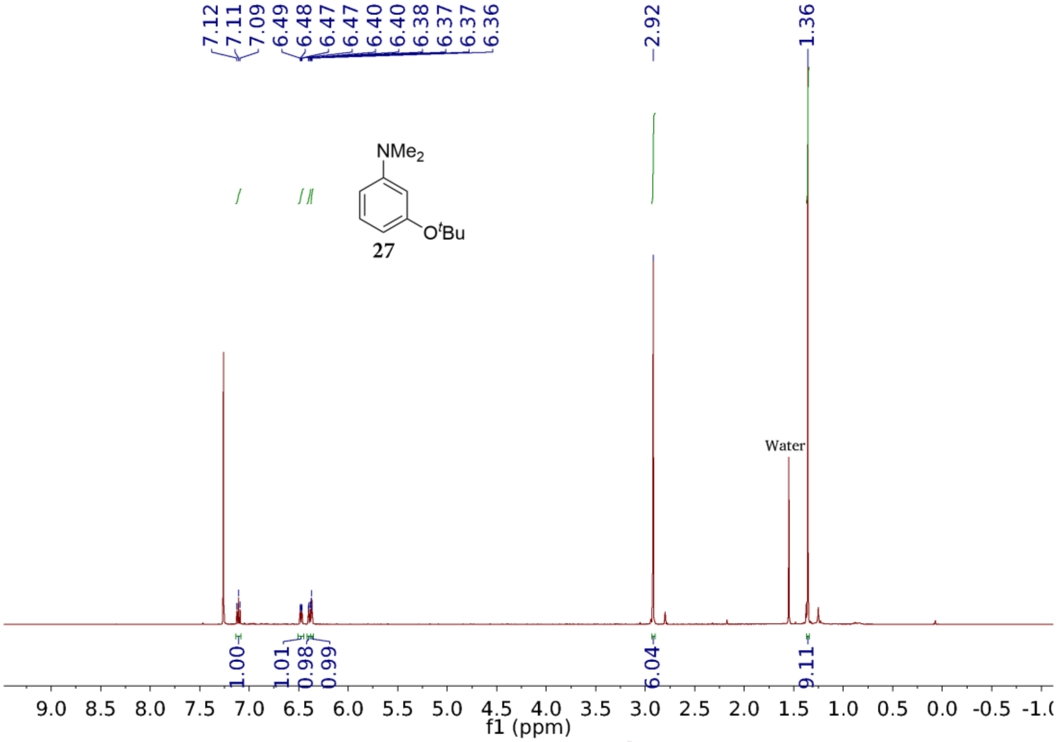

153.69
148.68
145.67
113.36
112.71
108.21
80.18
56.58
55.83
28.82
OMe
O^{t}Bu
OMe
21
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

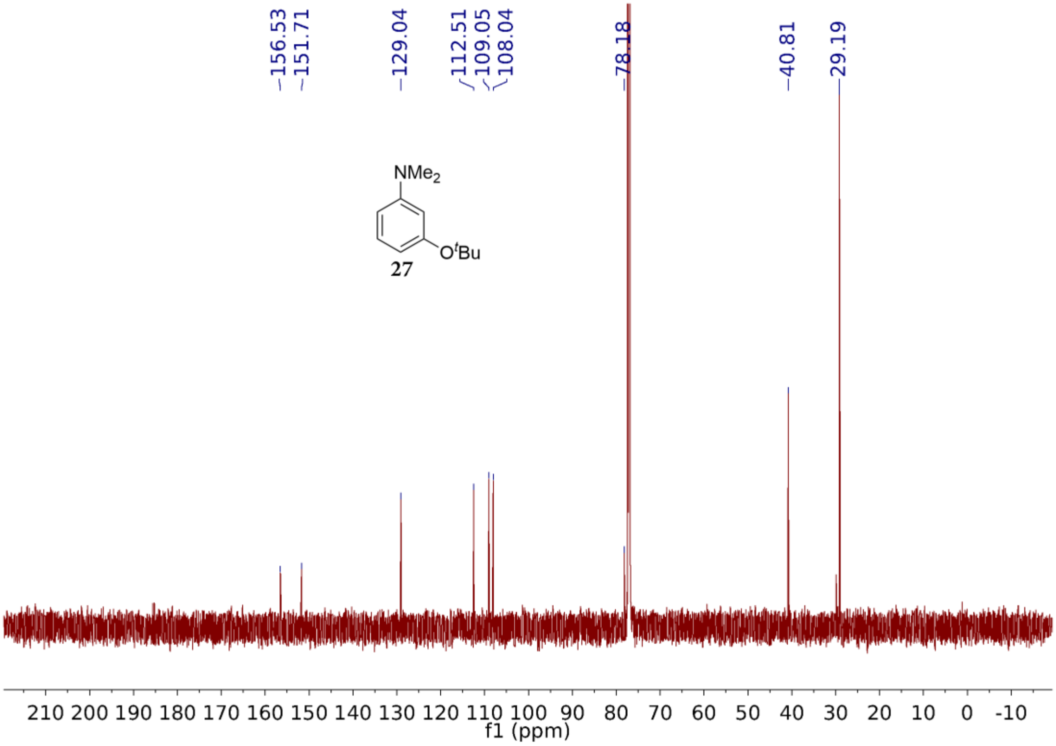

6.75
6.73
6.55
6.53
6.53
3.84
3.83
1.32
OMe
MeO
O^tBu
23
1.00
1.98
2.96
2.99
9.09
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)

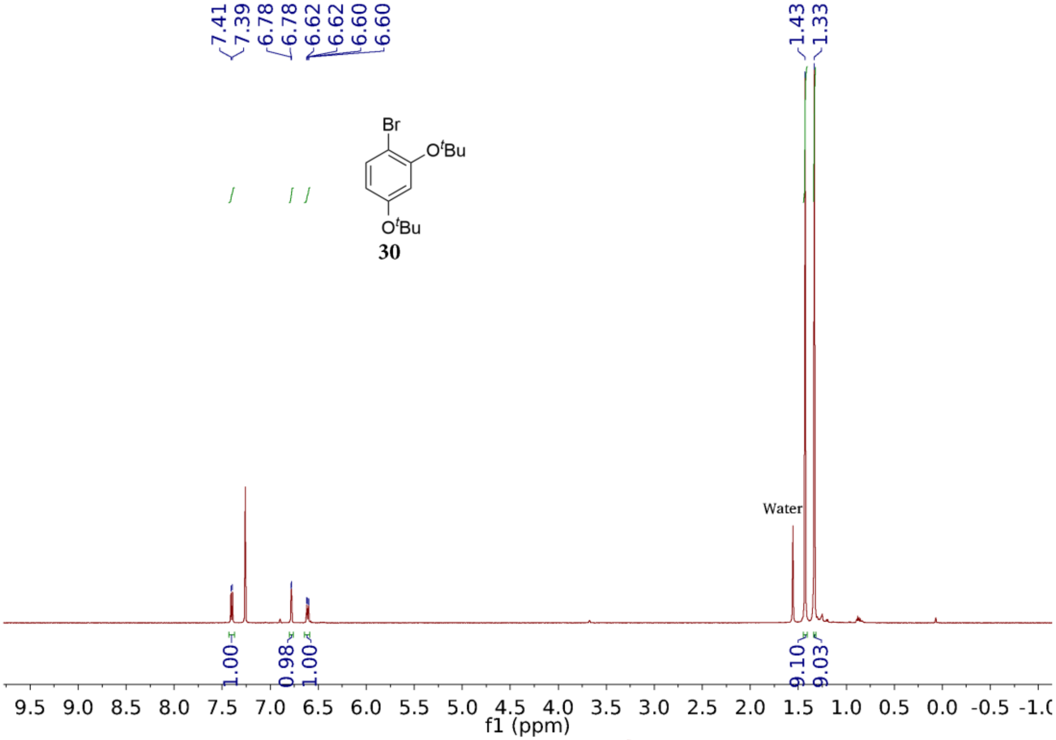

149.06
148.89
145.48
115.71
110.94
109.03
78.42
56.20
55.96
28.91
OMe
MeO
O^tBu
23
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

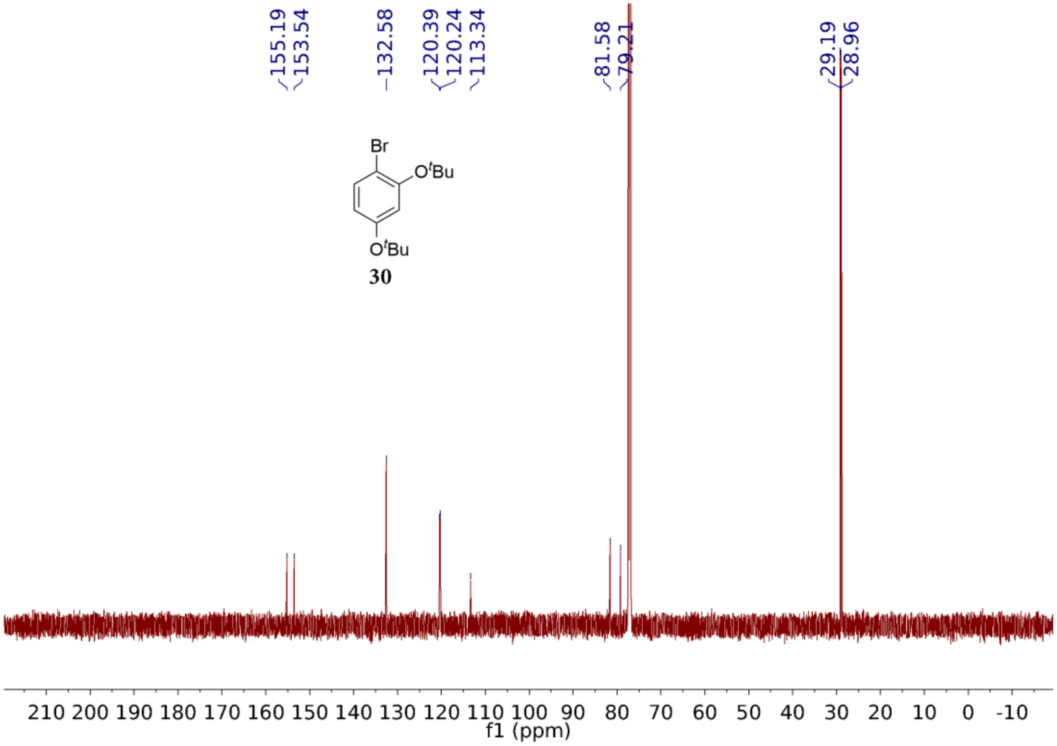

7.14
7.12
7.11
6.74
6.74
6.73
6.72
6.66
6.65
6.65
1.33
O^{t}Bu
O^{t}Bu
25
Water
1.00
2.00
1.00
18.12
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

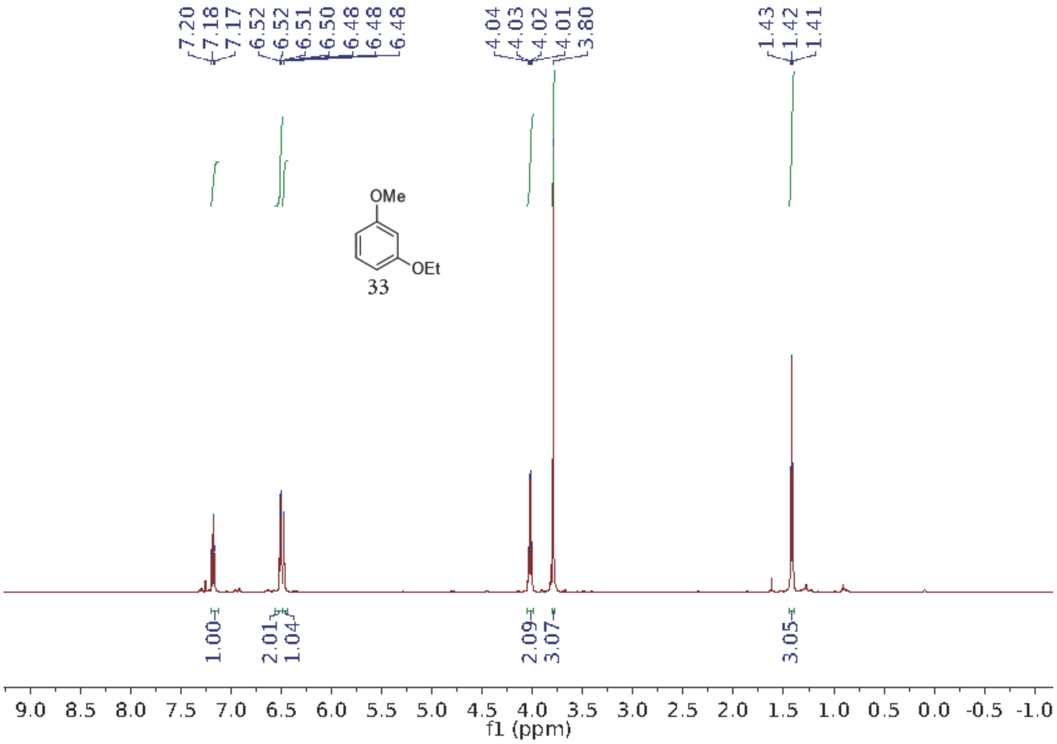

155.76
128.25
120.33
119.34
78.50
28.85
O^{t}Bu
O^{t}Bu
25
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

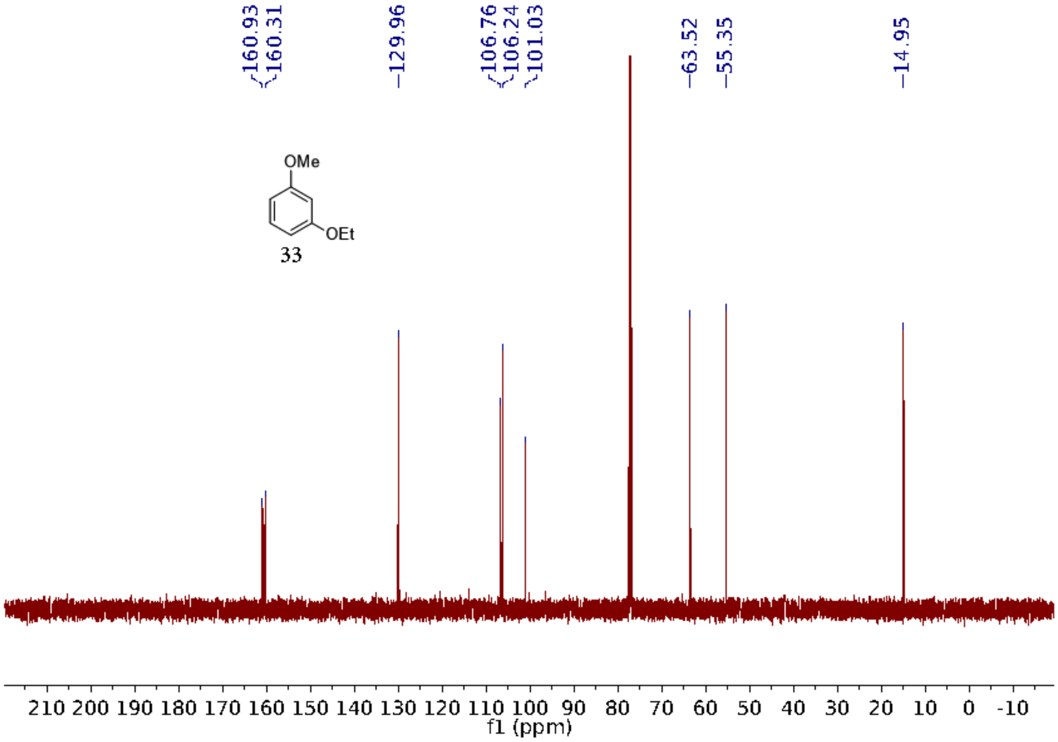

7.12
7.11
7.09
6.49
6.48
6.47
6.47
6.40
6.40
6.38
6.37
6.37
6.36
2.92
1.36
NMe2
O^tBu
27
Water
1.00
1.01
0.98
0.99
6.04
9.11
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

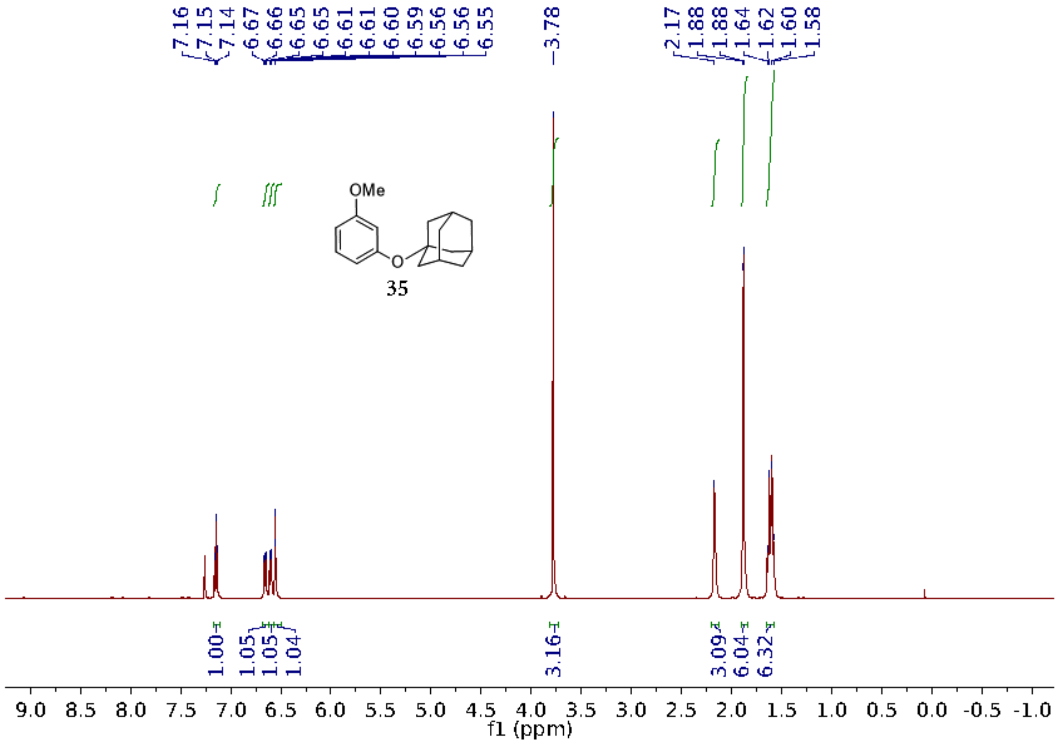

156.53
151.71
129.04
112.51
109.05
108.04
78.18
40.81
29.19
NMe2
O^tBu
27
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

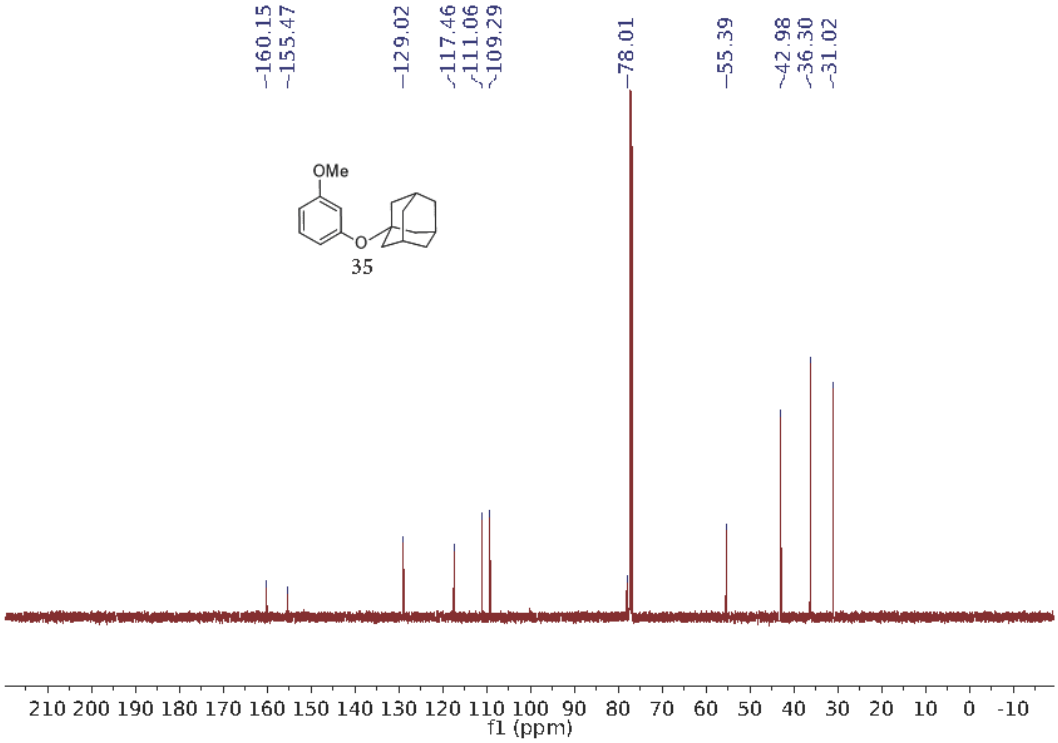

7.41
7.39
6.78
6.78
6.62
6.62
6.60
6.60
1.43
1.33
Br
O^{t}Bu
O^{t}Bu
30
Water
1.00
0.98
1.00
9.10
9.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

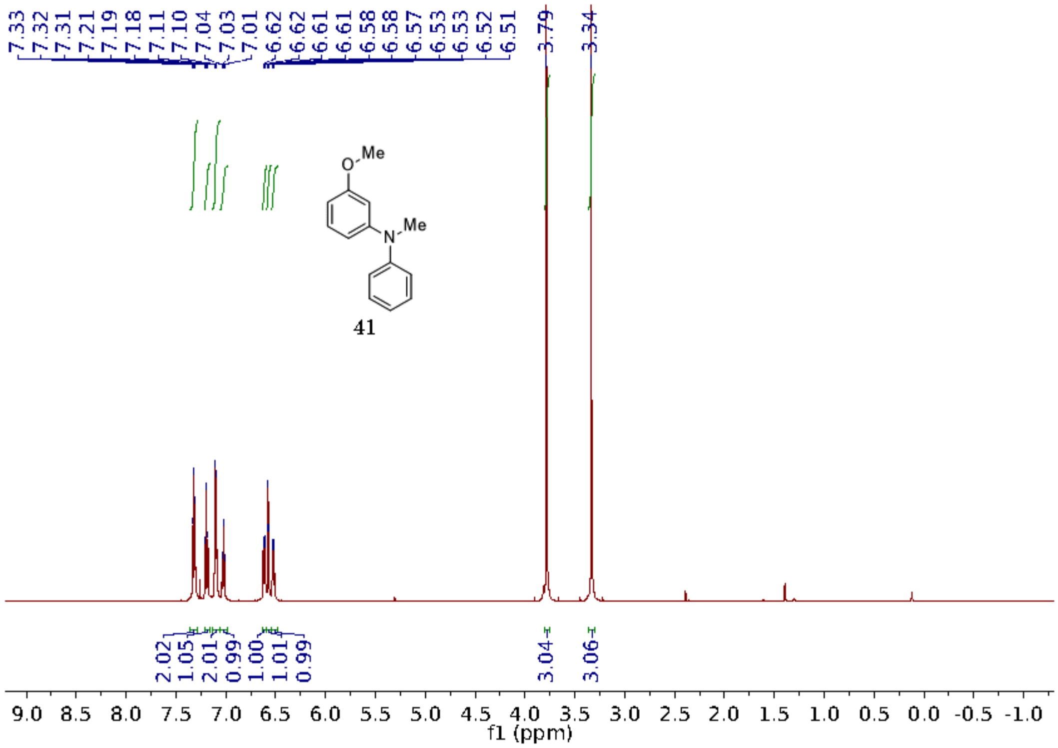

155.19
153.54
132.58
120.39
120.24
113.34
81.58
79.21
29.19
28.96
Br
O^{t}Bu
O^{t}Bu
30
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

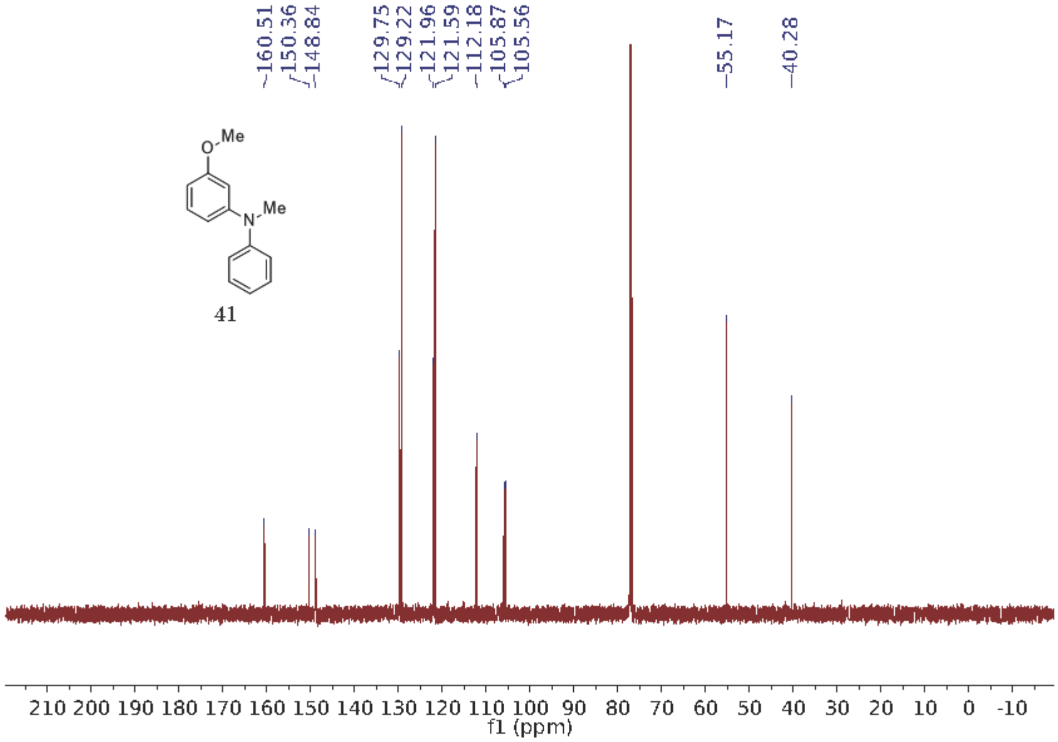

7.20
7.18
7.17
6.52
6.52
6.51
6.50
6.48
6.48
6.48
4.04
4.03
4.02
4.01
3.80
1.43
1.42
1.41
OMe
OEt
33
1.00
2.01
1.04
2.09
3.07
3.05
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


160.93
160.31
129.96
106.76
106.24
101.03
63.52
55.35
14.95
OMe
OEt
33
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.16
7.15
7.14
6.67
6.66
6.65
6.65
6.61
6.61
6.60
6.59
6.56
6.56
6.55
3.78
2.17
1.88
1.88
1.64
1.62
1.60
1.58
OMe
O
35
1.00
1.05
1.05
1.04
3.16
3.09
6.04
6.32
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


160.15
155.47
129.02
117.46
111.06
109.29
78.01
55.39
42.98
36.30
31.02
OMe
O
35
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)





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